

Fast and accurate solution of the Poisson equation in an immersed setting

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Abstract

We present a fast and accurate algorithm for the Poisson equation in complex geometries, using regular Cartesian grids. We consider a variety of configurations, including Poisson equations with interfaces across which the solution is discontinuous (of the type arising in multi-fluid flows). The algorithm is based on a combination of the Correction Function Method (CFM) and Boundary Integral Methods (BIM). Interface and boundary conditions can be treated in a fast and accurate manner using boundary integral equations, and the associated BIM. Unfortunately, BIM can be costly when the solution is needed everywhere in a grid, *e.g.* fluid flow problems. We use the CFM to circumvent this issue. The solution from the BIM is used to rewrite the problem as a series of Poisson equations in rectangular domains — which requires the BIM solution at interfaces/boundaries only. These Poisson equations involve discontinuities at interfaces, of the type that the CFM can handle. Hence we use the CFM to solve them (to high order of accuracy) with finite differences and a Fast Fourier Transform based fast Poisson solver. We present 2D examples of the algorithm applied to problems involving boundary conditions over complex geometries (with 4th order accuracy), and to a Poisson equation with interfaces across which the solution is discontinuous (with 3rd order accuracy).

Keywords: Poisson equation, Correction Function Method, Gradient augmented level set method, High accuracy, Immersed Method, Embedded meshes

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1. Introduction.

In this paper we present a fast and accurate numerical algorithm to solve the Poisson equation in complex geometries, using regular Cartesian grids. The algorithm is based on the combination of the Correction Function Method (CFM) [1] and boundary integral formulations of the Laplace equation [2, 3]. It can be applied to a wide variety of problems that involve solving the Poisson equation, particularly those with interfaces across which jump conditions are prescribed for both the solution and its normal derivative. The solution to problems of this type is of fundamental importance in, for example, the description of fluid flows separated by interfaces (*e.g.* the interfaces between immiscible fluids, or fluids separated by a membrane).

Standard finite difference discretizations yield poor approximations in the vicinity of a discontinuity. The exception is when the discontinuity occurs exactly on top of grid nodes. In this situation, the discontinuity can be incorporated into the discretization, to maintain the accuracy of the numerical scheme. In practice, an interface across which a discontinuity occurs is rarely aligned with a Cartesian grid. The CFM is based on the idea of introducing a *correction function*, defined in a narrow band enclosing the interface — which includes the grid nodes surrounding the interface. This correction function is used to provide a smooth extension, across the interface, of the solution on each side. As discussed in [1], the CFM can be employed to solve the Poisson equation with an arbitrary immersed interface, across which the solution obeys appropriate jump conditions, in a regular Cartesian grid.

However, the CFM [1] imposes restrictions on the type of interface jump conditions that it allows, which are not (generally) satisfied by the problems that arise in applications. In this paper we show how to remove these restrictions. To do so we build on an idea introduced by Mayo [4] to replace the original problem by sub-problems, each of which can be solved with the CFM. A brief summary of the process, described in detail in §3, follows.

We write the solution as the sum of two components. The first component satisfies the Poisson problem in which the jump in the normal derivative across the interface is set to vanish. By construction this first problem can be solved using the CFM. The second component solves the “deficit” problem, a Laplace equation which takes care of the jumps in the normal derivatives at

the interface. This second problem can be solved using a boundary integral method (BIM) [2–4]. However, we do not use the BIM to compute the solution at every grid point, as this would be costly. Instead we use the potential densities (at the interface) from the BIM, to write a third problem which the second component satisfies, and which is of the type that can be solved with the CFM.

A final point is that the solution domain can be embedded into a rectangular box, with the boundary transformed into an interface. As a consequence, the linear algebraic systems that a finite difference discretization and the CFM produce, can be efficiently solved using FFT techniques. Effectively, the problem is reduced to: (i) solving two standard (no interfaces) Poisson problems in a box, with simple (*e.g.* Dirichlet) boundary conditions at the box boundary, and (ii) using a BIM to compute potential densities at the interfaces and the boundary.

The accuracy of the algorithm can be arbitrary, since (in principle) the BIM and the CFM can be implemented to any desired order of accuracy. Furthermore, with the exception of the integral equations, all other steps involve problems defined in rectangular domains, which can be solved very efficiently using Fast Fourier transform (FFT) methods.¹ Hence, the overall solution procedure is also fast, since the costliest steps involve fast solutions of boundary integral equations [5–7], and an FFT based fast Poisson solver.

There exists a vast literature on immersed methods for the Poisson equation and related problems. By immersed methods here we mean: methods where the entire solution domain (normally involving complex geometries) is immersed into a regular Cartesian grid or triangulation. In particular, the combination of boundary integral equations and immersed methods was introduced in the seminal work by Mayo [4, 8, 9]. Recent work of particular interest focuses on Kernel-Free Boundary Integral Methods [10]. This new class may offer better efficiency for 3-D problems. Some of the other well established methods include the work by Johansen and Collela [11], the Immersed Boundary Method [12, 13], the Immersed Interface Method [14–17], and the Ghost Fluid Method [18–23]. The finite element community has also made significant progress in developing new immersed methods. Among these, we can mention the work by Dolbow and Harari [24], the Extended Finite Element Method [25], the Virtual Node Method [26], the finite element

¹No spectral methods involved: The discrete linear equations can be solved with FFTs.

versions of the Immersed Interface Method [27–30], and the Exact Subgrid Interface Correction Method [31].

The remainder of the paper is organized as follows. In §2 the general Poisson problem that we seek to solve is introduced. §3 includes the details of the proposed algorithm, as well as a discussion of issues such as accuracy and computational cost. §4 presents examples of the algorithm applied to examples involving complex geometries and interfaces of discontinuity. Finally, §5 contains the conclusions.

2. Definition of the problem

Throughout this paper, $\vec{x} = (x_1, x_2, \dots) \in \mathbb{R}^\nu$ is the spatial vector (where $\nu = 2$ or $\nu = 3$), Δ is the Laplace operator defined by

$$\Delta = \sum_{i=1}^{\nu} \frac{\partial^2}{\partial x_i^2}, \quad (1)$$

and Ω is an arbitrary, bounded and open, simply connected domain in \mathbb{R}^ν . This domain is split into two sub-domains, Ω^+ and Ω^- , by a co-dimension 1 surface Γ disjoint from the boundary $\partial\Omega$. The situation we have in mind is best described by a picture: see figure 1(a).

Let \hat{n} denote the unit vector normal to Γ , pointing towards Ω^+ and let u be a function defined in a neighborhood of Γ . Then

$$u_n = \hat{n} \cdot \vec{\nabla} u = \hat{n} \cdot (u_{x_1}, u_{x_2}, \dots) \quad \text{for } \vec{x} \in \Gamma \quad (2)$$

denotes the derivative of u in the direction of \hat{n} . Similarly, \hat{m} and u_m denote the outer normal vector to the boundary $\partial\Omega$, and the corresponding directional derivative.

Our objective is to solve the following Poisson problem

$$\beta^+ \Delta u(\vec{x}) = f^+(\vec{x}) \quad \text{for } \vec{x} \in \Omega^+, \quad (3a)$$

$$\beta^- \Delta u(\vec{x}) = f^-(\vec{x}) \quad \text{for } \vec{x} \in \Omega^-, \quad (3b)$$

where the jump conditions

$$[u] = a(\vec{x}) \quad \text{for } \vec{x} \in \Gamma, \quad (4a)$$

$$[\beta u_n] = b(\vec{x}) \quad \text{for } \vec{x} \in \Gamma, \quad (4b)$$

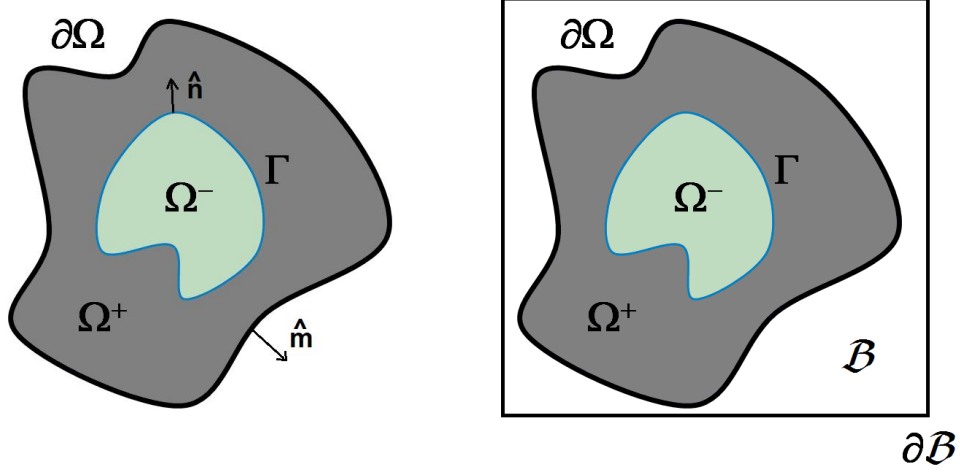


Figure 1: (a) Typical solution domain Ω , split by an internal interface Γ across which the solution and the equation parameters can jump. Note that there is no problem with allowing Ω^- to have more than one component. (b) The box \mathcal{B} enclosing Ω .

apply across the interface Γ . Here β^\pm are positive constants, f^\pm are some given functions² defined in Ω^\pm , a and b are known functions defined on Γ , and the brackets define the jump in the enclosed quantity across Γ

$$[*] = *^+ - *^-, \quad (5)$$

where the superscripts indicate on which side of Γ the quantity must be evaluated.

We consider either a Dirichlet or Neumann boundary conditions on the boundary $\partial\Omega$

$$u(\vec{x}) = g_D(\vec{x}) \quad \text{for } \vec{x} \in \partial\Omega, \quad (6a)$$

$$\text{or} \quad u_m(\vec{x}) = g_N(\vec{x}) \quad \text{for } \vec{x} \in \partial\Omega, \quad (6b)$$

where g_D or g_N are some given functions. In the case of a Neumann boundary condition (6b), we further assume that the compatibility condition

$$\int_{\Omega} f dV = \int_{\partial\Omega} g_N dS - \int_{\Gamma} b dS \quad (7)$$

²How smooth these functions need to be is tied up to how accurate an approximation is desired, *e.g.* for a 4th order algorithm, they have to be C^2 .

is satisfied.

Remark 1. In the literature the case when $\beta^+ = \beta^-$ is often called the *constant coefficients* case, while $\beta^+ \neq \beta^-$ is referred to as the *variable coefficients* case. We find this nomenclature a bit confusing, particularly the use of the word “variable” which suggests a function $\beta = \beta(\vec{x})$, not just two constants. ♣

Remark 2. The solution to (3–4) with Neumann boundary conditions (6b) is defined up to an arbitrary additive constant. There is a number of techniques that can be used to make the solution unique [3, 4, 32]. Here we do this by imposing an additional integral constraint, see §3.2. ♣

Remark 3. The Correction Function Method (CFM) [1] was developed to deal with interface conditions of the form in (4), for the case when $\beta^- = \beta^+$. The CFM offers a framework to solve problems of this type, to high order of accuracy, using finite differences on a regular Cartesian grid.

The CFM is based on the computation of a *correction function*, defined in the vicinity of Γ , which can be used to produce smooth extensions of u^\pm across Γ . These extensions can, in turn, be used to complete finite difference discretizations of the Laplace operator, without loss of accuracy, for stencils that straddle Γ . Furthermore, this process produces a discretized linear system whose coefficient matrix is the same as the one that arises when there is no interface. The systems only differ in their right hand sides. Hence the same linear solvers that work for “standard” Poisson problems can be used. Finally, the correction function is defined as the solution to a PDE problem and, in theory, can be computed to arbitrary order of accuracy. In [1] we show a 4th order implementation of the CFM, which is the same one that we use here to obtain the results presented in §4. ♣

2.1. The large β ratio limit.

Many applications in multiphase flows involve the solution of problems like the one above, with a large ratio between the coefficients β^\pm — which are the reciprocal of the densities. For example, for air–water interfaces the ratio is $\approx 10^3$. As we will demonstrate, the solution method presented in §3 is general enough to deal with such ratios, and larger.

However, the situation where $\beta^-/\beta^+ \gg 1$ involves a subtlety. In the limit $\beta^-/\beta^+ \rightarrow \infty$, equation (4b) yields $u_n^- = 0$. Thus u^- becomes the

solution to a Poisson problem in Ω^- , with a Neumann boundary condition on $\Gamma = \partial\Omega^-$. Hence u^- is defined only up to an arbitrary additive constant. For this reason, when β^-/β^+ is large, the Poisson problem in (3–4) can become poorly conditioned. Note that this issue is intrinsic to the problem being solved, and independent of which numerical algorithm is used.

There are situations where this poor conditioning does not arise. For example, some problems naturally demand an additional constraint to define a unique solution, such as: (i) Neumann boundary conditions (6b) are used, or (ii) Ω has a shape (*e.g.* a rectangle) that allows the use of periodic boundary conditions. In these cases, an appropriate choice of the extra constraint can yield a problem which is well conditioned for all values of β^-/β^+ . On the other hand, when Dirichlet conditions (6a) are used, no additional constraint is required for uniqueness. In this situation the value of β^-/β^+ has a direct impact on the conditioning of the problem. In appendix Appendix A we discuss a possible fix that can be used in the context of the solution method in §3.

3. Solution method

Here we introduce an algorithm to solve the problem introduced in §2. As discussed in §1, we do this by combining the Correction Function Method (CFM) [1] with the ideas introduced by Mayo [4, 8].

We start by splitting the solution into two components: $u = v + w$. The first component, v , is selected as the solution to a Poisson problem that can be solved with the CFM — see remark 3. The second component, w , then solves the “deficit” problem — the boundary and jump conditions that the CFM cannot handle in a direct fashion. The main objective of this section is to show how to solve this second problem.

An additional, and very important step, is to embed the domain Ω into a box \mathcal{B} — see figure 1(b). In this setting, $\partial\Omega$ is treated as an internal interface, playing a role similar to that of Γ . This step leads to a situation where the problems that need to be solved numerically are “standard” Poisson problems in the box \mathcal{B} . Hence the discretized systems can be inverted very efficiently using the Fast Fourier Transform (FFT).

The first component, v , is defined as the solution to the following Poisson

problem

$$\Delta v(\vec{x}) = \begin{cases} 0 & \text{for } \vec{x} \in \mathcal{B}/\Omega, \\ f^+(\vec{x})/\beta^+ & \text{for } \vec{x} \in \Omega^+, \\ f^-(\vec{x})/\beta^- & \text{for } \vec{x} \in \Omega^-, \end{cases} \quad (8a)$$

$$[v] = \begin{cases} a(\vec{x}) & \text{for } \vec{x} \in \Gamma, \\ 0 & \text{for } \vec{x} \in \partial\Omega, \end{cases} \quad (8b)$$

$$[v_n] = 0 \quad \text{for } \vec{x} \in \{\Gamma, \partial\Omega\}, \quad (8c)$$

$$v(\vec{x}) = 0 \quad \text{for } \vec{x} \in \partial\mathcal{B}. \quad (8d)$$

Note that here the jump condition in (4b) has been replaced by (8c), which makes the problem for v one for which “effectively”

- (i) The corresponding β^\pm and b satisfy $\beta^+ = \beta^- = 1$ and $b = 0$.
- (ii) The corresponding f^\pm and a follow from the right hand sides in (8a) and (8b).

Thus, by construction, this is a problem that can be solved using the CFM — see remark 3. In addition, by taking care of the forcing terms f^\pm and the jump function a , these equations guarantee that the “deficit” system for w is a Laplace equation problem with a boundary integral formulation — as shown in theorems 1 and 2.

The equations for w follow by subtracting (8) from (3–6)

$$\Delta w(\vec{x}) = 0 \quad \text{for } \vec{x} \in \Omega, \quad (9a)$$

$$[w] = 0 \quad \text{for } \vec{x} \in \Gamma, \quad (9b)$$

$$[\beta w_n] = b(\vec{x}) - [\beta v_n] \quad \text{for } \vec{x} \in \Gamma, \quad (9c)$$

with

$$w(\vec{x}) = g_D(\vec{x}) - v(\vec{x}) \quad \text{for } \vec{x} \in \partial\Omega, \quad (10a)$$

$$\text{or } w_m(\vec{x}) = g_N(\vec{x}) - v_m(\vec{x}) \quad \text{for } \vec{x} \in \partial\Omega. \quad (10b)$$

In the discussion that follows, it is convenient to rewrite (9c) in terms of $[w_n]$. To accomplish this, we use the following identity

$$[pq] = \langle p \rangle [q] + [p] \langle q \rangle, \quad (11)$$

where

$$\langle * \rangle = \frac{*^+ + *^-}{2} \quad (12)$$

denotes the mean value across a discontinuity of the enclosed quantity. Using (11) and (8c) in (9c), we obtain the alternative form

$$[w_n] + \lambda \langle w_n \rangle = b(\vec{x}) / \langle \beta \rangle - \lambda v_n(\vec{x}) \quad \text{for } \vec{x} \in \Gamma, \quad (9c)$$

where $\lambda = [\beta] / \langle \beta \rangle$. Below we show how to solve (9–10) using a combination of Mayo’s method [4] and the CFM. We address the cases with Dirichlet and Neumann boundary conditions separately, in §3.1 and §3.2 resp.

3.1. Dirichlet boundary conditions

An efficient approach to solve (9–10) is to use a boundary integral formulation, in which the solution is written as a combination of convolution integrals of the fundamental solution to the Laplace equation, and potentials defined along Γ and $\partial\Omega$. The following theorem is appropriate for the Dirichlet case.

Theorem 1. *Let $\rho \in C^1(\Gamma)$ and $\mu \in C^1(\partial\Omega)$ be the solution to the following system of integral equations*

$$\begin{aligned} \rho(\vec{x}) + \frac{\lambda}{2\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS \\ + \frac{\lambda}{2\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_{nm}(\vec{x}, \vec{x}_s) dS = \frac{b}{\langle \beta \rangle} - \lambda v_n \end{aligned} \quad \text{for } \vec{x} \in \Gamma, \quad (13a)$$

$$\begin{aligned} \mu(\vec{x}) + \frac{1}{\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \\ + \frac{1}{\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS = 2(g_D(\vec{x}) - v(\vec{x})) \end{aligned} \quad \text{for } \vec{x} \in \partial\Omega, \quad (13b)$$

where \vec{x}_s denotes the position vector along the integration surface, and Φ is the fundamental solution of the Laplace equation.³ Then, the solution of the problem in (9), with the Dirichlet boundary condition in (10a), is given by

$$\begin{aligned} w(\vec{x}) = \frac{1}{2\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \\ + \frac{1}{2\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS \end{aligned} \quad \text{for } \vec{x} \in \mathcal{B}. \quad (14)$$

³In 2-D, $\Phi(\vec{x}, \vec{x}_s) = \log(|\vec{x} - \vec{x}_s|)$; and in 3-D, $\Phi(\vec{x}, \vec{x}_s) = \frac{1}{|\vec{x} - \vec{x}_s|}$ — see [33].

The proof is given in appendix Appendix B. ♣

In theorem 1, ρ is known as the monopole or single layer potential, while μ is known as the dipole or double layer potential. These potential functions are commonly used in the solution of the Laplace equation with a boundary integral formulation [2, 3, 33]. Furthermore, (13) is a Fredholm integral equation of the second kind, as is normally the case with the Laplace equation. This class of integral equations has been extensively studied and there is a number of well established numerical methods — Boundary Integral Methods (BIM) — that we can use to solve for the potentials [2, 3]. Nevertheless, although the potentials can be computed accurately and efficiently, to obtain the solution in Ω the convolution integrals in (14) need to be evaluated. This last step can be relatively expensive when the solution is needed at a large number of points. In addition, the fundamental solution of the Laplace equation is singular on the boundary and the interfaces, which makes evaluating the solution even more expensive in the vicinity of these surfaces. These difficulties can be circumvented by computing the solution inside Ω using finite differences, as proposed by Mayo [4] and described below.

Equation (14) defines a solution valid everywhere in \mathbb{R}^n , including the box \mathcal{B} . Hence, we can use (14) to evaluate the solution on the boundary of \mathcal{B} , and define an equivalent Poisson problem in \mathcal{B} with a Dirichlet boundary condition. Furthermore, the solution described by (14) is discontinuous across Γ and $\partial\Omega$, with the jumps in the solution and its normal derivative directly related to the local value of the potentials — *e.g.* see [3]. It follows that w is the solution to the following problem

$$\Delta w(\vec{x}) = 0 \quad \text{for } \vec{x} \in \mathcal{B}, \quad (15a)$$

$$[w] = \begin{cases} 0 & \text{for } \vec{x} \in \Gamma, \\ -\mu(\vec{x}) & \text{for } \vec{x} \in \partial\Omega, \end{cases} \quad (15b)$$

$$[w_n] = \begin{cases} \rho(\vec{x}) & \text{for } \vec{x} \in \Gamma, \\ 0 & \text{for } \vec{x} \in \partial\Omega, \end{cases} \quad (15c)$$

$$w(\vec{x}) = \frac{1}{2\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS + \frac{1}{2\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_{n_s}(\vec{x}, \vec{x}_s) dS \quad \text{for } \vec{x} \in \partial\mathcal{B}. \quad (15d)$$

This problem is, again, of the type that can be solved using the CFM. Furthermore, it is also a problem in the box \mathcal{B} , so that the discretized system

can be inverted very efficiently using the FFT.

The rectangular domain \mathcal{B} is arbitrary. However, to reduce the number of grid points outside the region of interest, \mathcal{B} should enclose Ω as tightly as possible. On the other hand, evaluating (15d) too close to $\partial\Omega$ is difficult. Hence, for practical reasons, the distance from $\partial\Omega$ to $\partial\mathcal{B}$ should not be too small. In our calculations we used the distance of three grid spacings suggested by Mayo [4].

Finally, note that (13a) involves evaluating normal derivative v_n along Γ . In general, we expect v_n to be one order less accurate than the nominal accuracy of the CFM. Furthermore, since the solution to (13) determines the jump conditions in (15),

$$\textit{the solution } u \textit{ is one order less accurate than the CFM accuracy.} \quad (16)$$

For instance, with a 4th order accurate CFM, v_n can be computed along Γ with 3rd order accuracy only. The potentials are then restricted to 3rd order accuracy, and thus so are w and $u = v + w$.

Remark 4. The CFM requires knowledge of the jump functions at a number of points along the interfaces. The location of these points depends both on implementation details and on the way that the Cartesian grid is located relative to the interfaces. In (15) the jump conditions are given by the solution to (13) that results from using a BIM. Some BIM output potential distributions defined all along the interfaces (*e.g.* Galerkin’s method). However, most BIM output potential values on a finite number of nodes along the interfaces. In these cases interpolation is needed to compute the values at the points required by the CFM. For the examples in this paper, we solved 2-D problems with uniformly distributed quadrature nodes, and used an FFT based trigonometric interpolation [34]. ♣

Remark 5. The BIM requires a discretization of Γ and $\partial\Omega$. However, these discretizations are completely independent from the finite differences computational grid used to solve (8) and (15). In fact, it is quite possible to have a BIM which is more accurate than the finite difference scheme. In this case the discretization used for Γ and $\partial\Omega$ can be much coarser than the grid used to solve (8) and (15). ♣

Remark 6. Since (8) and (15) are solved in a rectangular domain, and the CFM modifications occur only on the right hand side of the discretized system

(see remark 3), the FFT can be used to solve the linear system that arises from the finite difference discretization. This fact makes this approach very cost effective.⁴ ♣

Remark 7. There is not a unique way to compute v_n along Γ . However, since we can use the correction function to extend the solution across the discontinuity interface, it is convenient to adopt a formulation that is consistent with the CFM [1]. In the CFM, the correction function is represented using Hermite polynomials — with degree depending on the desired accuracy. Therefore, we also represent v in the vicinity of Γ by Hermite polynomials defined in each cell of the grid that straddles Γ . From this v_n can be computed by differentiating a polynomial. Furthermore, although v is discontinuous, v_n is continuous across Γ — see (8c). Thus v_n can be computed using the Hermite polynomial representation for either v^+ or v^- . ♣

3.2. Neumann boundary conditions

The solution process for this case is quite similar to the one discussed in §3.1. The appropriate boundary integral formulation is now the one given by theorem 2.

Theorem 2. Let $\rho_1 \in C^1(\Gamma)$ and $\rho_2 \in C^1(\partial\Omega)$ be the solution to the following system of integral equations

$$\begin{aligned} \rho_1(\vec{x}) + \frac{\lambda}{2\pi} \int_{\Gamma} \rho_1(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS \\ + \frac{\lambda}{2\pi} \int_{\partial\Omega} \rho_2(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS = \frac{b}{\langle\beta\rangle} - \lambda v_n \end{aligned} \quad \text{for } \vec{x} \in \Gamma, \quad (17a)$$

$$\begin{aligned} \rho_2(\vec{x}) + \frac{1}{\pi} \int_{\Gamma} \rho_1(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS \\ + \frac{1}{\pi} \int_{\partial\Omega} \rho_2(\vec{x}_s) (1 + \Phi_m(\vec{x}, \vec{x}_s)) dS = 2(g_N(\vec{x}) - v_m(\vec{x})) \end{aligned} \quad \text{for } \vec{x} \in \partial\Omega, \quad (17b)$$

⁴Note that this does not involve using spectral methods. The FFT can be used to invert the linear system because finite difference discretizations of the Laplace operator produce circular periodic linear systems.

where \vec{x}_s denotes the position vector along the integration surface, and Φ is the fundamental solution of the Laplace equation. Then

$$\begin{aligned} w(\vec{x}) = & \frac{1}{2\pi} \int_{\Gamma} \rho_1(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \\ & + \frac{1}{2\pi} \int_{\partial\Omega} \rho_2(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \end{aligned} \quad \text{for } \vec{x} \in \mathcal{B} \quad (18)$$

is the solution of the problem in (9), with the Neumann boundary condition in (10b), plus the additional constraint

$$\int_{\partial\Omega} \rho_2 dS = 0. \quad (19)$$

The proof is given in appendix Appendix B. ♣

Just as in §3.1, (17) is a Fredholm integral equation of the second kind, which can be solve (to find ρ_1 and ρ_2) by using a well established BIM. Then, after the potentials are known, w follows by solving the following problem

$$\Delta w(\vec{x}) = 0 \quad \text{for } \vec{x} \in \mathcal{B}, \quad (20a)$$

$$[w] = 0 \quad \text{for } \vec{x} \in \{\Gamma, \partial\Omega\}, \quad (20b)$$

$$[w_n] = \begin{cases} \rho_1(\vec{x}) & \text{for } \vec{x} \in \Gamma, \\ \rho_2(\vec{x}) & \text{for } \vec{x} \in \partial\Omega, \end{cases} \quad (20c)$$

$$\begin{aligned} w(\vec{x}) = & \frac{1}{2\pi} \int_{\Gamma} \rho_1(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \\ & + \frac{1}{2\pi} \int_{\partial\Omega} \rho_2(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \end{aligned} \quad \text{for } \vec{x} \in \partial\mathcal{B}. \quad (20d)$$

As before, this problem can be solved using the CFM, with the resulting linear system inverted efficiently using the FFT — see remark 6.

3.3. Main algorithm

The method described in §3.1 and §3.2 is summarized by the algorithm below

1. Define the computational domain \mathcal{B} and create the Cartesian grid.
2. Discretize Γ and $\partial\Omega$ — see remark 5.
3. **if** $f \neq 0$ or $a \neq 0$ **then**

4. Solve problem (8), and find v , using the CFM [1].
5. Compute v_n on Γ (at the quadrature points used to discretize the surface integrals) — see remark 7.
6. **end if**
7. Solve the boundary integral equation (13) or (17) with a BIM (obtain the potentials) — see, for example, refs. [2–4]
8. Interpolate the potentials at the nodes required by the CFM — see remark 4.
9. Solve problem (15) or (20), and find w , using the CFM [1].
10. Set $u = v + w$.

3.4. General remarks

The algorithm presented in this section can be readily applied to problems where there is no interface Γ , to reduce a formulation over an irregular domain to one in a box \mathcal{B} , which can then be solved very efficiently. In these situations, the interface Γ is absent from the problem, and the expressions in (8) to (20) remain valid as long as the terms involving Γ are removed. Furthermore, the absence of Γ implies that there is no need to compute v_n along Γ to determine w . Thus, the reason behind the loss of accuracy in (16) is absent, and the method then recovers the full CFM accuracy.

Extensions to more general problems involving the Poisson equation are also feasible — including external problems with finite support, as long as there exists a boundary integral formulation to solve the Laplace equation with the corresponding interface and boundary conditions — the analog of (9). The general algorithm involves the steps listed below.

1. **“Constant coefficient” component.** Define a problem that can be directly addressed by the CFM, and such that it produces a Laplace equation “deficit” system. That is, set the jumps in the normal derivatives to zero, as done in the problem for v in (8). As explained there, this gives rise to a “constant coefficients” problem (*i.e.* $\beta^+ = \beta^-$) which can be solved with the CFM in the first step of the process.
In addition, embed the solution domain Ω into a box \mathcal{B} , and convert the boundary $\partial\Omega$ into an interface by (i) setting the source term to zero in \mathcal{B}/Ω , and (ii) assuming trivial interface jump conditions on $\partial\Omega$. Finally, use trivial boundary conditions on $\partial\mathcal{B}$. This yields a problem that the CFM can reduce to a linear system solvable with FFT techniques.

2. **“Discontinuous coefficient” and immersed boundaries component** — that is, the “deficit” problem for $w = u - v$, where v is the solution found in part 1, and u is the solution to the full problem. By construction the function w satisfies Laplace’s equation problem, with the appropriate interface and boundary conditions. The solution to this problem can be split into four sub-steps:
 - (a) Write the corresponding boundary integral formulation.
 - (b) Find the potential distributions for the integral formulation using a BIM.
 - (c) Write an equivalent Laplace equation system in \mathcal{B} , in such a way that it can be solved using the CFM. That is, use the potential distributions obtained with the BIM to write appropriate jump conditions across Γ and $\partial\Omega$.
 - (d) Solve this equivalent Laplace equation system using the CFM and FFT.
3. **Full solution.** The complete solution is given by the sum of the two components above.

Next we consider the issue of accuracy. Four factors are important

1. **Representation of interfaces and boundaries.** The interface and boundary conditions must be enforced with accuracy compatible with the rest of the algorithm. This, in turn, requires accurately knowing the position of the interfaces and boundaries. For the examples in §4 we use the Gradient Augmented Level Set Method (GALSM) [35], which allows tracking of the geometry to 4th order of accuracy using local grid information.
2. **Accuracy of the BIM.** The accuracy of these methods depends on the smoothness of the interfaces, the boundaries, and of the data provided on these surfaces. For smooth and well resolved surfaces, Nystrom’s method is guaranteed to converge as fast as the quadrature rule used to approximate the integrals [3].
3. **Interpolation of the potential distributions.** As pointed out in remark 4, interpolation of the solution given by the BIM, to the points required by the CFM, is needed. In this paper the example applications are in 2-D, with smooth geometries. Thus we use trigonometric interpolation [34], which can be efficiently computed using the FFT, and has optimal accuracy.

4. **The accuracy of the CFM.** There is no “in principle” limit to the CFM accuracy [1], provided that the data (source terms and jump functions) is smooth enough. In our examples we use a 4th order implementation.

The overall accuracy of the algorithm proposed here is determined by the least accurate of the factors listed above. Since, in principle, each of these factors can be made as accurate as needed; there is no inherent limit to the algorithm order.

Finally, let us consider the issue of the cost of the algorithm proposed here. For this purpose, let us assume that (i) in the BIM interfaces and boundaries are discretized using a total of k nodes, and (ii) the finite differences discretization of the computational domain involves M nodes.⁵ Then the break down of the computational costs is as follows (recall that the space dimension is ν)

1. **Cost of the BIM.** The cost of the BIM depends on the specific choice of method. In principle, a general BIM requires $\mathcal{O}(k^3)$ operations. However, there is a number of techniques that can be used to reduce this cost to $\mathcal{O}(k^2)$ or even to $\mathcal{O}(k)$, see [5–7].
2. **Cost of computing the boundary conditions.** In equations (15) and (20) integrations are needed to evaluate the boundary conditions. The integration cost for each node on the boundary is $\mathcal{O}(k)$, so that the total cost of evaluating the boundary conditions is $\mathcal{O}(kM^{(\nu-1)/\nu})$.
3. **Interpolation costs.** As pointed out in remark 4, interpolation of the potential functions obtained with the BIM may be required. Depending on the technique used, the cost of computing interpolants for the potential distributions varies between $\mathcal{O}(k)$ and $\mathcal{O}(k^2)$. After the interpolants are known, the cost of evaluating the potentials at the locations needed by the CFM is $\mathcal{O}(M^{(\nu-1)/\nu})$.
4. **Cost of the CFM.** Computing the correction function requires the solution of a small linear system (12×12 for 4th order accuracy in 2-D) at each grid node close to the interface or the boundary. The total cost for this is $\mathcal{O}(M^{(\nu-1)/\nu})$. However, note that these linear systems depend on the geometry of the problem only — thus their coefficient matrices need to be computed only once. As a consequence, even though the

⁵Recall that the two discretizations are independent of each other — see remark 5.

CFM is used more than once to obtain the full solution, the additional cost incurred over a single use is rather minimal.

5. **Cost of the finite differences.** Since all the problems solved with finite differences are defined in a rectangular domain, the resulting linear systems can be inverted using the FFT. This is one of the fastest methods available to solve the Poisson equation, with cost $\mathcal{O}(M \log M)$.

Remark 8. Mayo and collaborators [4, 8, 9] proposed a method similar to the one here, for the Laplace and Poisson equations without interfaces of discontinuity. As here, their method uses a BIM and finite differences in an immersed setting. They also considered the case with discontinuities, which they do by adding correction terms to the right hand side of the discretized equations. However, instead of using the CFM, the correction terms are based on accurate computations of derivatives of the potentials. Fourth order accurate corrections for the Laplace equation are presented in [4, 8], and second order corrections for the Poisson equation in [9]. ♣

4. Results

Here we present three examples of computations in 2-D using the algorithm proposed in §3. In the first example we consider the problem of imposing Dirichlet and Neumann conditions on an immersed boundary (example with no interfaces). In the second example we solve a Poisson problem, in open space, with an interface at which the solution is discontinuous (example with no boundaries). Finally, in the third example we consider a combination of the previous two: a Poisson problem with a discontinuity interface and Dirichlet conditions at an immersed boundary. In the examples with a discontinuity interface we show results for situations where the ratio of the β coefficients is very large: 10^6 . The algorithm presented in §3 combines several numerical methods, each of which has several possible variants. The specific variants used for the calculations presented in this section are as follows

- For the boundary integral equation we use Nystrom’s method with the trapezoidal quadrature rule [3–5]. For smooth interfaces and data, this method has optimal convergence and accuracy.
- For the potential distributions we use FFT based trigonometric interpolants [34] — see remark 4.

- Interfaces and boundaries immersed in regular Cartesian grids are represented using the Gradient-Augmented Level-Set Method [35]. This provides 4th order accuracy using local grid information.
- The Laplace and Poisson equations are discretized to 4th order accuracy using the standard 9-point stencil [1]. The CFM correction function is computed to 4th order accuracy using the implementation in ref. [1].

Nystrom’s method converges rapidly for problems involving smooth data, such as the examples below. However, to interpolate potential functions over immersed boundaries and interfaces, a reasonable number of points is needed to guarantee accuracy. In principle the discretization of the interface used by Nystrom’s method should be refined as the Cartesian grid is refined, so that the interpolation errors do not become dominant. Here, for simplicity, we use a single discretization, with equally spaced nodes, in each of the examples below.⁶ For the Cartesian grids used, this proved sufficient to make the interpolation errors insignificant, even at the finest resolution.

4.1. Example 1. Boundary conditions in a complex geometry

Let Ω be the region contained within the zero contour of ϕ :

$$\phi(x, y) = r^2 - r_d^2, \quad (21a)$$

$$\text{where } r = \sqrt{x^2 + y^2}, \quad (21b)$$

$$r_d = r_0 + \delta \sin(5\theta), \quad (21c)$$

$$\theta = \tan^{-1} \left(\frac{y}{x} \right), \quad (21d)$$

$r_0 = 1$, and $\delta = 0.3$. For this domain, consider the Poisson equation associated with the exact solution $u(x, y) = \cos(x) \sin(y)$, with either Dirichlet or Neumann boundary conditions. The solution to the problem with Neumann boundary conditions is made unique by the constraint in (19) — see remark 2 — and differs from u by an additive constant only.

Figure 2(a) shows Ω immersed in a regular Cartesian discretization of a square box. The black line in figure 2(a) is the boundary $\partial\Omega$ (the the zero

⁶The precise numbers are: Example 1: 500 nodes for the boundary. Example 2: 200 nodes for the “boundary” and 400 nodes for the interface. Example 3: 200 nodes for the boundary and 400 nodes for the interface.

contour of ϕ). Figure 2(b) shows a plot of the solution, obtained with the Dirichlet boundary condition in a refined grid. Note that the algorithm sets the solution outside Ω to zero.

Figure 3 illustrates the convergence of the method: error (both in the L_∞ and L_2 norms) as a function of the Cartesian grid spacing $h = \Delta x = \Delta y$. For both the Dirichlet and Neumann problems, the norms indicate 4th order convergence (as expected). Furthermore, the error in the L_∞ norm has similar size in both cases.

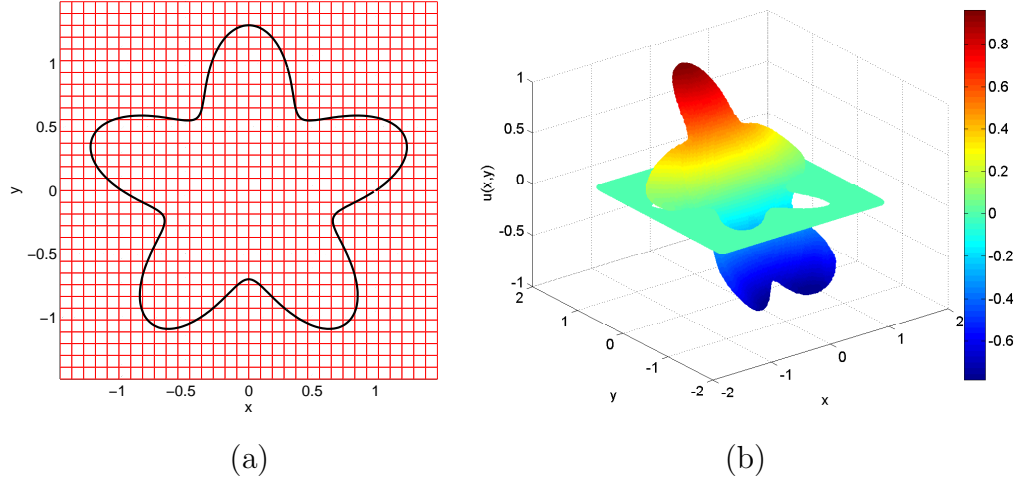


Figure 2: (a) Solution domain Ω for example 1, embedded into a 33×33 Cartesian grid. (b) Dirichlet boundary conditions solution, obtained with a 193×193 grid.

4.2. Example 2. Poisson problem in open space with a large β^\pm ratio discontinuity interface

In this example we solve the Poisson problem (3), with interface jump conditions (4), associated with the exact solution

$$u^+(x, y) = \exp(-r^2/0.0008), \quad (22a)$$

$$u^-(x, y) = \cos(x) \sin(y) + 1.5, \quad (22b)$$

and

$$\beta^+ = 10^6, \quad \beta^- = 1,$$

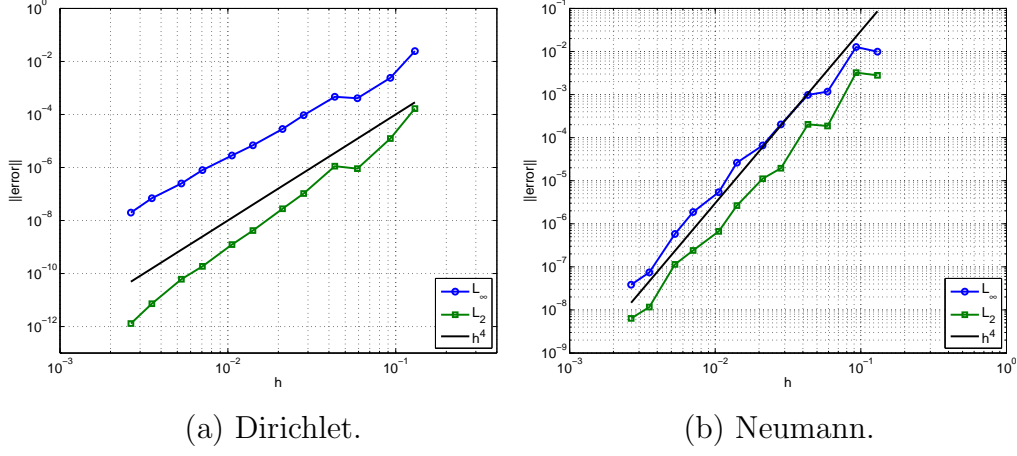


Figure 3: Error for example 1, as a function of the grid spacing h , for the Dirichlet (left) and Neumann (right) cases. L_∞ norm in blue, L_2 norm in green, and h^4 in black.

where r is defined in (21). The discontinuity interface Γ is defined as the zero contour of ϕ in (21), with parameters $r_0 = 0.1$ and $\delta = 0.03$ — see the solid black line in figure 4(a).

The solution to this problem is defined everywhere in \mathbb{R}^2 , and it decays fast enough, as $r \rightarrow \infty$, that it effectively vanishes outside the 1×1 box \mathcal{B} shown in figure 4(a) — *e.g.* $|u| < 1 \times 10^{-15}$ for $r > 0.4$. Thus we use this box as the computational domain.

However, which boundary conditions should we use? The fact that the solution effectively vanishes for $r > 0.4$ is misleading. If the solution truly vanished there, then

$$\int_{\mathbb{R}^2/\mathcal{B}} \Delta u \, dx \, dy = 0$$

would apply. However, it is easy to check that

$$\left| \int_{r>0.4} \Delta u \, dx \, dy \right| > 2.4.$$

Hence any boundary condition based on the naive assumption that the solution is identically zero outside the box \mathcal{B} would introduce significant changes, invalidating (22) as the “exact” solution. We circumvent this problem by creating an additional interface at $r = 0.4$ — the dashed line in figure 4(a). Here we then enforce appropriate jump conditions that yield $u \equiv 0$ for $r > 0.4$.

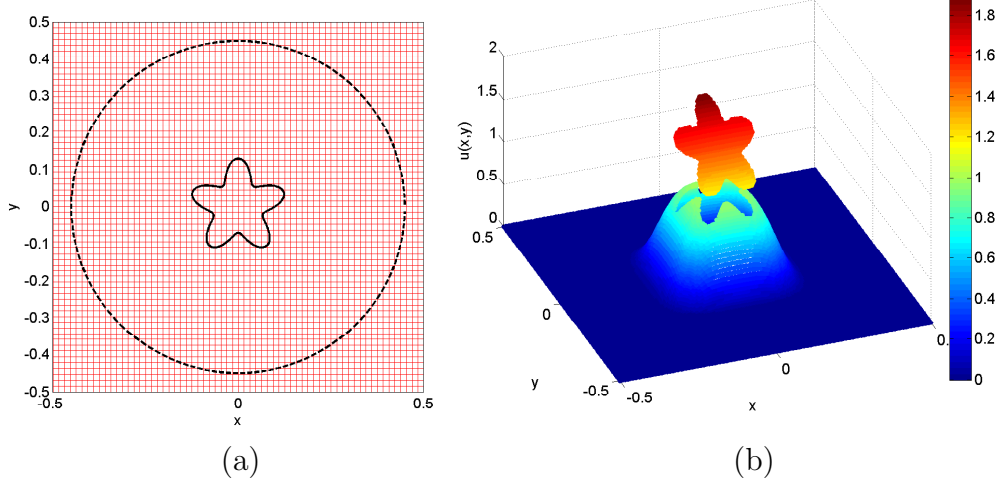


Figure 4: (a) The 1×1 computational box \mathcal{B} used in example 2. The dashed line is the circle of radius $r = 0.4$, and the solid black line the interface Γ . An embedding Cartesian grid is also shown. (b) Solution obtained with a 193×193 grid.

These jump conditions are not known a priori, but may be obtained after the first step of the algorithm, *i.e.*, the solution v of the Poisson problem in (8).

Figure 4(b) shows a plot of the solution obtained with this technique, while figure 5 illustrates the convergence of the method — both in the L_∞ and L_2 norms. As expected, see (16), 3rd order convergence occurs.

4.3. Example 3. Poisson problem with Dirichlet conditions on an immersed boundary and a large β^\pm ratio discontinuity interface

In this example we solve the Poisson problem (3), with interface jump conditions (4), associated with the exact solution

$$u^+(x, y) = r^2 = x^2 + y^2, \quad (23a)$$

$$u^-(x, y) = \cos(x) \sin(y) + 2, \quad (23b)$$

with the choices of coefficients β^\pm in (25). The solution domain Ω is the unit disk, with boundary $\partial\Omega$ represented by the zero contour of

$$\psi = r^2 - 1. \quad (24)$$

The discontinuity interface Γ is defined as the zero contour of ϕ in (21), with parameters $r_0 = 0.5$ and $\delta = 0.1$. Figure 6(a) shows the solution domain

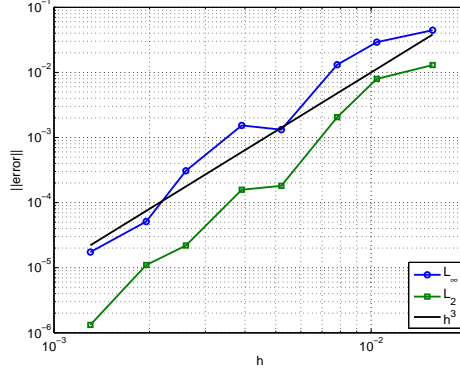


Figure 5: Error for example 2, as a function of the grid spacing h . L_∞ norm in blue, L_2 norm in green, and h^3 in black.

Ω , and the interface Γ , immersed in a regular Cartesian discretization of a square computational domain \mathcal{B} . Finally, we consider the following two situations for the coefficients β^\pm

$$(i) \beta^+ = 10^6 \text{ and } \beta^- = 1, \quad \text{or} \quad (ii) \beta^+ = 1 \text{ and } \beta^- = 10^6. \quad (25)$$

As pointed out in §2.1 (see appendix Appendix A for technical details), case (ii) yields a poorly conditioned problem. A straightforward application of the solution algorithm converges at the expected rate, but with a prefactor in the error that grows with the ratio β^-/β^+ . To overcome this problem, we use the simple fix proposed in appendix Appendix A. This requires enforcing an integral constraint that the solution is known to satisfy, which depends only on the problem's data. We select the mean value of the potential ρ in the integral equation (13), which for the current problem is given by

$$\langle \rho \rangle = 0.837801918284980. \quad (26)$$

Note that this value can be computed from the mean value of b over Γ , and the mean value of f^- in Ω^- . We call the solution obtained using this technique the “corrected solution.”

The solution using (25)(i), and the corrected solution using (25)(ii) are visually indistinguishable. Figure 6(b) shows a plot of the solution, using (25)(i), in a refined grid. The convergence of the method is displayed in figure 7 for both cases, (i) and (ii), using the L_∞ and L_2 norms. As expected,

see (16), the convergence is 3rd order. Figure 7(ii) includes the results for calculations done with, and without, the constraint in (26) — the corrected results are shown using solid lines. Notice that, while the convergence is 3rd order for both the corrected and the uncorrected calculations, the errors for the corrected case have roughly the same size as those for the case using (25)(i), while the errors for the uncorrected case are, approximately, 10^6 times bigger. This number is directly related to the condition number of boundary integral equation being solved, which in turn is related to the ratio between the β^\pm coefficients — see §2.1 and appendix Appendix A.

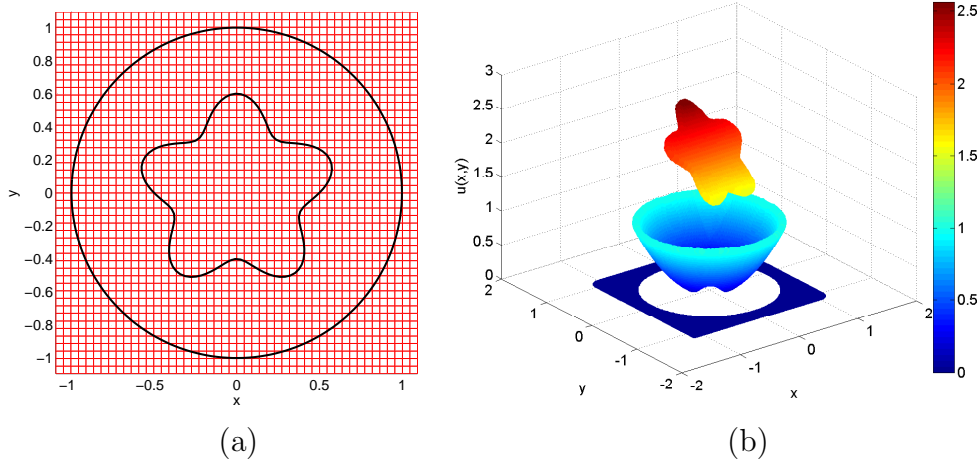


Figure 6: (a) Solution domain Ω for example 3, embedded in a 33×33 Cartesian Grid. The boundary $\partial\Omega$, and the discontinuity interface Γ , are shown by solid black lines. (b) Solution obtained with a 193×193 grid.

5. Conclusion

In this paper we presented an algorithm to solve the Poisson equation in arbitrarily shaped domains immersed in regular Cartesian grids. The algorithm can be applied to the Poisson equation in general settings, including interfaces across which the solution is discontinuous — with jumps in the solution and “weighted” normal derivatives prescribed. The algorithm relies on computationally efficient and accurate numerical methods.

The efficiency results from the fact that we split the problem into (i) a boundary integral equation, and (ii) one or two “constant coefficients”

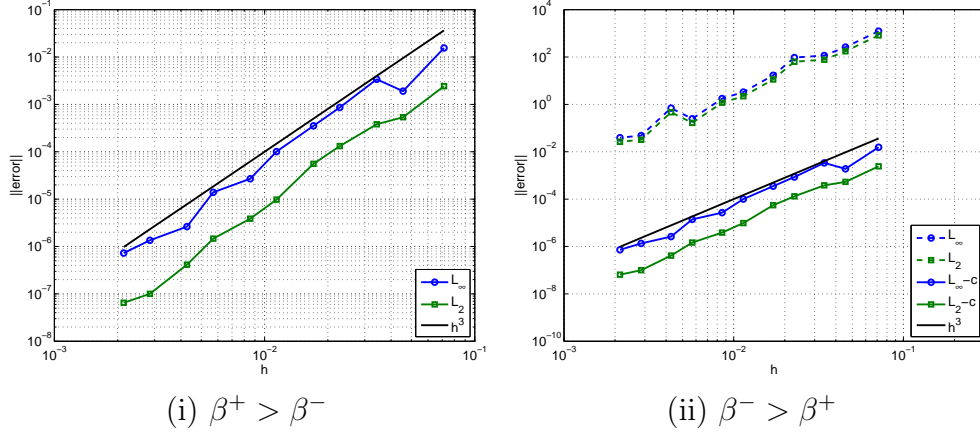


Figure 7: Error for example 3, as a function of the grid spacing h . L_∞ norm in blue, L_2 norm in green, and h^3 in black. For case (ii), $\beta^- > \beta^+$, the dashed lines are the errors for the calculations without the constraint in (26).

Poisson equations defined in rectangular domains.⁷ The boundary integral equation can be efficiently solved using well established boundary integral methods (BIM), whereas the Poisson equations are solved with finite differences and the Correction Function Method (CFM). The rectangular domains result in discretized linear systems that can be solved very efficiently using the Fast Fourier Transform (FFT).

A 3rd or 4th order of accuracy (depending on the type of boundary condition used) version of the algorithm was implemented, and used on several examples to illustrate the method. Note that, since the BIM and CFM may be implemented to any order of accuracy, there is no inherent limit to the accuracy that can be achieved with the method proposed here.

In principle the solution procedure presented here can be extended to 3-D. However, we have not yet implemented the current method in 3-D. The reason is that, while evaluating the integrals in eqs. (15d) and (20d) can be done very efficiently in 2-D, it is an efficiency bottleneck in 3-D. However, recent work in ref. [10] on the Kernel-Free Boundary Integral Method (KFBIM) provides a natural path for addressing this issue. Currently we are investigating the joint use of the CFM and the KFBIM for the purpose of obtaining a method

⁷The meaning that “constant coefficients” has in this context is explained in remark 1.

both high order (as the method in this paper), and also efficient in 3-D.

Appendix A. Remarks on conditioning

As discussed in §2.1, when $\alpha = \beta^-/\beta^+ \gg 1$ is large, the Poisson problem in (3–4) can become poorly conditioned. To understand this issue, we look at the jump condition for the normal fluxes — equation (4b)

$$\begin{aligned} \beta^+ u_n^+(\vec{x}) - \beta^- u_n^-(\vec{x}) &= b(\vec{x}) \\ \Rightarrow u_n^+(\vec{x}) - \alpha u_n^-(\vec{x}) &= \frac{b(\vec{x})}{\beta^+} \end{aligned} \quad \text{for } \vec{x} \in \Gamma. \quad (\text{A.1})$$

Assuming that both u_n^+ and b/β^+ are $\mathcal{O}(1)$ quantities, in the limit $\alpha \rightarrow \infty$, we obtain $u_n^- \rightarrow 0$. Hence, in this limit (A.1) becomes a Neumann boundary condition for u^- . Thus the solution for u^- decouples from u^+ . Furthermore, u^+ becomes the solution to the problem with the Dirichlet boundary condition $u^+(\vec{x}) = a(\vec{x}) - u^-(\vec{x})$ for $\vec{x} \in \Gamma$.

From the arguments above, it follows that u^- is determined only up to an arbitrary constant “in the limit” $\alpha = \infty$, while u^+ follows uniquely once u^- is known. In situations where the full problem requires an extra constraint to define a unique solution,⁸ this is not an issue — the constraint selects a unique u^- . By contrast, when Dirichlet boundary conditions on $\partial\Omega$ apply, the solution to the full problem is unique (for any finite value of α), without any constraints being needed. Yet, in the limit $\alpha \rightarrow \infty$ this uniqueness is lost. The numerical evidence indicates that this loss of uniqueness is tied up to the condition number for the problem going to infinity as $\alpha \rightarrow \infty$.

Note that *the poor conditioning arising when $\alpha \gg 1$ does not occur as a consequence of any particular numerical method used to solve the equations. It is, in fact, inherent to the problem itself.* Hence, in order to improve the conditioning when $\alpha \gg 1$, the problem itself must be modified, somehow. An “obvious” fix is to enforce an additional constraint. However, since the solution is uniquely determined, the additional constraint must be redundant. It should be there only to “reinforce” information that is weakly enforced due to the imbalance between the different terms in (A.1) when α is large.

For example, within the context of the algorithm discussed in §3, the issue surfaces in the Laplace problem in (9) — specifically in (9c), which causes this

⁸For example, when Neumann conditions on $\partial\Omega$ apply.

system to become poorly conditioned for $\alpha = \beta^-/\beta^+ \gg 1$ and the Dirichlet boundary conditions in (10a). In turn, we may readily verify that, in the limit $\alpha \rightarrow \infty$ the integral operator acting on ρ in (13a) is the same as the one that arises with a Neumann boundary condition. This integral operator is well known to have a one-dimensional nullspace, whose generator has a non-zero mean — see [2, 3, 33].

We can improve the conditioning of the equation by enforcing an adequate mean value for the monopole potential ρ in the associated boundary integral equation (13), as explained below.

Therefore, we can define a unique solution to the integral equation (13) by adding a constraint on the mean value of ρ to (13a). For more details, see Appendix B.

Second, let us show that the mean value of ρ over Γ is defined only by known parameters of the problem. We start by noting that $\rho = [w_n]$ — see (8). In fact, since w is the solution to a Laplace equation, the divergence theorem implies that

$$\int_{\Gamma} w_n^- dS = 0 \quad (\text{A.2})$$

and thus

$$\int_{\Gamma} \rho dS = \int_{\Gamma} [w_n] dS = 2 \int_{\Gamma} \langle w_n \rangle dS. \quad (\text{A.3})$$

Then, we integrate (9c) to obtain

$$\int_{\Gamma} \rho dS = \frac{2}{\lambda + 2} \left(\frac{1}{\langle \beta \rangle} \int_{\Gamma} b dS - \lambda \int_{\Gamma} v_n dS \right). \quad (\text{A.4})$$

Next, we recur once more to the divergence theorem and (8) to write

$$\int_{\Gamma} v_n dS = \frac{1}{\beta^-} \int_{\Omega^-} f^- dV. \quad (\text{A.5})$$

Finally, we can replace (A.5) into (A.4) to obtain the following expression.

$$\int_{\Gamma} \rho dS = \frac{2}{\lambda + 2} \left(\frac{1}{\langle \beta \rangle} \int_{\Gamma} b dS - \frac{\lambda}{\beta^-} \int_{\Omega^-} f^- dV \right). \quad (\text{A.6})$$

Expression (A.4) reinforces the reason why the problem is poorly conditioned. As α grows, λ approaches the value $\lambda = -2$. Hence, the mean value of ρ becomes very sensitive to any errors in the data, especially those coming from the computation of v_n .

One way to force the numerical scheme to “see” the proper mean of ρ is to enforce (A.6) as the extra condition and input the correct value to the code. Note that, in principle we can compute the correct value using (A.6) since it only involves known parameters of the problem: b and f^-/β^- . However, because of the $(\lambda+2)$ term in the denominator, we must be able to compute the integrals in (A.6) very accurately, which may not always be easy to do. In the example shown in §4.3, we integrated this expression using the trapezoidal rule and were able to obtain very accurate estimates. One may hope that in real applications physical reasoning might help to deduce the correct value for the mean of ρ . (We did not encounter a physical problem that leads to this particular situation). Finally, there may be other ways to enforce a redundant condition that is more suitable to the particular problem being solved. Using (A.6) is just one alternative that we found to work when the integrals can be computed accurately.

Appendix B. Proof of theorems 1 and 2

Proof of theorem 1. The proof relies on well established properties of the Laplace equation and its fundamental solution. These properties are discussed in many textbooks dedicated to this subject, *e.g.* [2, 3, 33], so we will reproduce these results without proof.

Let us write the solution to (9) as $w = w_1 + w_2$ with

$$w_1(\vec{x}) = \frac{1}{2\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \quad \text{for } \vec{x} \in \mathcal{B}, \quad (\text{B.1a})$$

$$w_2(\vec{x}) = \frac{1}{2\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS \quad \text{for } \vec{x} \in \mathcal{B}. \quad (\text{B.1b})$$

Both w_1 and w_2 satisfy the Laplace equation everywhere in \mathbb{R}^ν . Then, all we need to complete the proof is to show that w satisfies the jump conditions (9b)-(9c) and the boundary condition (10a). For that, let us take limits of

(B.1a) to evaluate w_1 and its normal derivative on both sides of Γ :

$$w_1^+(\vec{x}) = \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega^+}} w_1(\vec{x}^*) = \frac{1}{2\pi} \int_{\Gamma}^{\text{PV}} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \quad \text{for } \vec{x} \in \Gamma, \quad (\text{B.2a})$$

$$w_1^-(\vec{x}) = \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega^-}} w_1(\vec{x}^*) = \frac{1}{2\pi} \int_{\Gamma}^{\text{PV}} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \quad \text{for } \vec{x} \in \Gamma, \quad (\text{B.2b})$$

$$\begin{aligned} \frac{\partial^+}{\partial \hat{n}}(w_1(\vec{x})) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega^+}} \frac{\partial}{\partial \hat{n}} w_1(\vec{x}^*) \\ &= \frac{1}{2} \rho(\vec{x}) + \frac{1}{2\pi} \int_{\Gamma}^{\text{PV}} \rho(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS \end{aligned} \quad \text{for } \vec{x} \in \Gamma, \quad (\text{B.2c})$$

$$\begin{aligned} \frac{\partial^-}{\partial \hat{n}}(w_1(\vec{x})) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega^-}} \frac{\partial}{\partial \hat{n}} w_1(\vec{x}^*) \\ &= -\frac{1}{2} \rho(\vec{x}) + \frac{1}{2\pi} \int_{\Gamma}^{\text{PV}} \rho(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS \end{aligned} \quad \text{for } \vec{x} \in \Gamma, \quad (\text{B.2d})$$

where PV denotes the principal value of the integral. As direct consequence of (B.2), w_1 satisfies $[w_1] = 0$, $[w_{1_n}] = \rho(\vec{x})$ for $\vec{x} \in \Gamma$. Similarly, we can take limits of (B.1b) to evaluate w_2 and its normal derivative on both sides of $\partial\Omega$:

$$\begin{aligned}
w_2^+(\vec{x}) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \mathcal{B}/\Omega}} w_2(\vec{x}^*) \\
&= -\frac{1}{2}\mu(\vec{x}) + \frac{1}{2\pi} \int_{\partial\Omega}^{\text{PV}} \rho(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS
\end{aligned}
\quad \text{for } \vec{x} \in \partial\Omega, \quad (\text{B.3a})$$

$$\begin{aligned}
w_2^-(\vec{x}) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega}} w_2(\vec{x}^*) \\
&= \frac{1}{2}\mu(\vec{x}) + \frac{1}{2\pi} \int_{\partial\Omega}^{\text{PV}} \mu(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS
\end{aligned}
\quad \text{for } \vec{x} \in \partial\Omega, \quad (\text{B.3b})$$

$$\begin{aligned}
\frac{\partial^+}{\partial \hat{m}}(w_2(\vec{x})) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \mathcal{B}/\Omega}} \frac{\partial}{\partial \hat{m}} w_2(\vec{x}^*) \\
&= \frac{1}{2\pi} \int_{\partial\Omega}^{\text{PV}} \mu(\vec{x}_s) \Phi_{mn}(\vec{x}, \vec{x}_s) dS
\end{aligned}
\quad \text{for } \vec{x} \in \partial\Omega, \quad (\text{B.3c})$$

$$\begin{aligned}
\frac{\partial^-}{\partial \hat{m}}(w_2(\vec{x})) &= \lim_{\substack{\vec{x}^* \rightarrow \vec{x} \\ x^* \in \Omega}} \frac{\partial}{\partial \hat{m}} w_2(\vec{x}^*) \\
&= \frac{1}{2\pi} \int_{\partial\Omega}^{\text{PV}} \mu(\vec{x}_s) \Phi_{mn}(\vec{x}, \vec{x}_s) dS
\end{aligned}
\quad \text{for } \vec{x} \in \partial\Omega. \quad (\text{B.3d})$$

It follows from (B.3) that $[w_2] = -\mu(\vec{x})$ and $[w_{2_m}] = 0$ for $\vec{x} \in \partial\Gamma$.

Replacing (B.2) and (B.3) into the jump conditions and Dirichlet boundary condition results in the system of integral equations

$$\begin{aligned}
\rho(\vec{x}) + \frac{\lambda}{2\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi_n(\vec{x}, \vec{x}_s) dS \\
+ \frac{\lambda}{2\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_{nm}(\vec{x}, \vec{x}_s) dS &= \frac{b}{\langle \beta \rangle} - \lambda v_n
\end{aligned}
\quad \text{for } \vec{x} \in \Gamma, \quad (13a)$$

$$\begin{aligned}
\mu(\vec{x}) + \frac{1}{\pi} \int_{\Gamma} \rho(\vec{x}_s) \Phi(\vec{x}, \vec{x}_s) dS \\
+ \frac{1}{\pi} \int_{\partial\Omega} \mu(\vec{x}_s) \Phi_m(\vec{x}, \vec{x}_s) dS &= 2(g_D(\vec{x}) - v(\vec{x}))
\end{aligned}
\quad \text{for } \vec{x} \in \partial\Omega. \quad (13b)$$

Thus, if ρ and μ are the solution to (13), w is the solution to (9) with Dirichlet boundary condition (10a) and the proof is complete. \square

Proof of theorem 2. The proof in the Neumann case is very similar to the one for the Dirichlet case and we will omit the details. The only point worth

mentioning is the addition of the condition

$$\int_{\partial\Omega} \rho_2 dS = 0, \quad (19)$$

which is used to make the solution unique.

Define the integral operators

$$\mathcal{K}(\ast) = \int_{\partial\Omega} (\ast) \Phi_m dS \quad \text{and} \quad \mathcal{A}(\ast) = \int_{\partial\Omega} (\ast) dS.$$

The boundary integral formulation in (17) involves the term $(\pi + \mathcal{K})\rho_2$. The operator $\pi + \mathcal{K}$ has a 1-dimensional nullspace, which is related to the arbitrary additive constant that can be added to the solution to the problem with Neumann boundary conditions — see remark 2. However, let ψ be a generator of the nullspace. Then it can be shown that $\mathcal{A}\psi \neq 0$. Thus (19) added to (10b) defines a unique solution. Further, alternative, approaches are discussed in [3, 4, 32]. \square

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